

2-(Difluoromethoxy)-1,1,1,3,3,3-hexafluoropropane  
26103-08-2 | DTXSID60448843

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

## Model Results

**Predicted value:**  $3.74 \times 10^{-14}$  cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Inside

**Local applicability domain index:**  $6.80 \times 10^{-1}$

**Confidence level:**  $7.16 \times 10^{-1}$

## Nearest Neighbors from the Training Set

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2-(Difluoromethoxy)-1,1,1,3,3,3-hexafluoropropane

**Measured:**  $7.50 \times 10^{-14}$

**Predicted:**  $3.74 \times 10^{-14}$

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1,1,1,3,3,3-Hexafluoro-2-propanol

**Measured:**  $2.58 \times 10^{-14}$

**Predicted:**  $2.03 \times 10^{-14}$

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Isoflurane

**Measured:**  $1.51 \times 10^{-14}$

**Predicted:**  $2.12 \times 10^{-14}$

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Enflurane

**Measured:**  $1.19 \times 10^{-14}$

**Predicted:**  $1.24 \times 10^{-14}$